Integrative Structure Validation Report July 22, 2024 - 04:59 PM PDT

The following software was used in the production of this report:

Python-IHM Version 1.3 MolProbity Version 4.5.2 Integrative Modeling Validation Version 1.2

PDB ID	9A2I		
PDB-Dev ID	PDBDEV_00000167		
Structure Title Model of E. coli DnaK by in-cell photo-crosslinking MS and deep learning			
Structure Authors Stahl, K.; Graziadei, A.; Dau, T.; Brock, O.; Rappsilber, J.			

This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.

We welcome your comments at pdb-dev@mail.wwpdb.org

A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

List of references used to build this report is available here.

Overall quality o

This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: MolProbity Analysis



Ensemble information ?

This entry consists of 0 distinct ensemble(s).

Summary ?

This entry consists of 10 unique models, with 1 subunits in each model. A total of 1 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 1 flexible or non-rigid units.

Entry composition?

There are 10 unique types of models in this entry. These models are titled None, None respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	P0A6Y8	А	А	638
2	1	1	P0A6Y8	А	А	638
3	1	1	P0A6Y8	А	А	638
4	1	1	P0A6Y8	A	А	638
5	1	1	P0A6Y8	А	А	638
6	1	1	P0A6Y8	A	А	638
7	1	1	P0A6Y8	A	A	638
8	1	1	P0A6Y8	A	А	638
9	1	1	P0A6Y8	А	А	638
10	1	1	P0A6Y8	А	А	638

Datasets used for modeling @

There is 1 unique dataset used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Crosslinking-MS data	jPOSTrepo	JPST001851

Representation Image: Comparison of the second symplectic comparison of the second symplecti						
Chain ID Rigid bodies Non-rigid segments						
А	A - 1-638					

Methodology and software

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	AlphaLink with 10 msa subsamples	AlphaLink	None	10	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	AlphaLink	1.0	model building	https://github.com/lhatsk/AlphaLink



Crosslinking-MS

Validation for this section is under development.

Model quality ?

For models with atomic structures, molprobity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Standard geometry: bond outliers?

There are 48730 bond outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Bond type	Observed distance (Å)	ldeal distance (Å)	Number of outliers
CBHB2	1.09	0.97	4560
CBHB	1.09	0.97	1350
CEHE2	1.09	0.97	650
CG2HG22	1.09	0.97	1350
CBHB1	1.09	0.97	700
CG2HG23	1.09	0.97	1350
NZHZ2	1.01	0.89	500
CBHB3	1.09	0.97	4560
CD2HD23	1.09	0.97	480
CGHG2	1.09	0.97	2000
CGHG3	1.09	0.97	2000
CGHG	1.09	0.97	480
CD2HD22	1.09	0.97	480
CDHD2	1.09	0.97	980
CAHA	1.09	0.97	5910
CD1HD11	1.09	0.97	920
CG2HG21	1.09	0.97	1350
CDHD3	1.09	0.97	980
CEHE1	1.09	0.97	150
CG1HG12	1.09	0.97	910
CD2HD21	1.09	0.97	480
CD1HD12	1.09	0.97	920

Bond type	Observed distance (Å)	ldeal distance (Å)	Number of outliers
NZHZ1	1.01	0.89	500
CAHA2	1.09	0.97	470
CD1HD13	1.09	0.97	920
OG1HG1	0.96	0.84	440
CEHE3	1.09	0.97	650
NZHZ3	1.01	0.89	500
CAHA3	1.09	0.97	470
CG1HG13	1.09	0.97	910
CG1HG11	1.09	0.97	470
ОННН	0.96	0.84	70
OGHG	0.96	0.84	250
NH1	1.01	0.89	10
NH2	1.01	0.89	10
NH3	1.01	0.89	10
SGHG	1.33	1.20	2
SGHG	1.34	1.20	8
NH	1.01	0.86	6140
CE2HE2	1.08	0.93	220
NE2HE22	1.01	0.86	370
CD2HD2	1.08	0.93	300
CZHZ	1.08	0.93	150
CE1HE1	1.08	0.93	299
NH2HH22	1.01	0.86	250

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Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NEHE	1.01	0.86	250
CD1HD1	1.08	0.93	230
NE2HE21	1.01	0.86	370
NH1HH11	1.01	0.86	250
ND2HD21	1.01	0.86	260
NH2HH21	1.01	0.86	250
NH1HH12	1.01	0.86	250
ND2HD22	1.01	0.86	260
CH2HH2	1.08	0.93	10
ND1HD1	1.01	0.86	75
CZ3HZ3	1.08	0.93	10
NE1HE1	1.01	0.86	10
CE3HE3	1.08	0.93	10
CZ2HZ2	1.08	0.93	10
NE2HE2	1.01	0.86	4
CE1HE1	2.09	0.93	1
NE2HE2	2.14	0.86	1

Standard geometry: angle outliers?

There are 457 angle outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Angle type	Angle type Observed angle (°)		Number of outliers
ND1-CE1-NE2	108.40	56.55	1
CD2-NE2-CE1	109.00	65.72	1
CG-CD2-NE2	107.20	78.03	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
C-N-CA	121.70	156.89	1
C-N-CA	121.70	150.36	1
CA-C-N	116.20	141.48	1
CA-C-N	116.20	140.95	1
O-C-N	123.00	103.74	1
O-C-N	123.00	105.29	1
CG-ND1-CE1	109.30	127.10	1
C-N-CA	121.70	140.13	1
CA-N-CD	112.00	100.33	1
CA-CB-CG	113.80	121.80	1
N-CA-C	111.00	132.65	1
C-CA-CB	110.50	122.01	1
CA-CB-CG	112.60	120.26	1
CA-CB-CG	112.60	120.24	1
C-N-CA	121.70	135.20	1
C-N-CA	121.70	135.03	1
CA-CB-CG1	110.40	122.96	1
N-CA-C	111.00	131.16	1
C-N-CA	121.70	133.98	1
CA-CB-CG	113.80	120.54	1
CB-CG-CD2	131.20	122.45	1
C-N-CA	121.70	133.70	1
C-N-CA	121.70	133.56	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
OE1-CD-NE2	122.60	116.04	1
C-N-CA	121.70	133.15	1
CA-C-N	116.90	126.43	1
C-CA-CB	111.40	123.46	1
C-CA-CB	110.50	119.85	1
CA-CB-OG1	109.60	118.94	1
N-CA-CB	110.50	99.96	1
OG1-CB-CG2	109.30	121.66	1
C-N-CA	121.70	132.67	1
C-N-CA	121.70	132.65	1
C-N-CA	121.70	132.54	1
CB-CG-CD2	131.20	123.39	1
OD1-CG-ND2	122.60	116.62	1
OE1-CD-NE2	122.60	116.69	1
C-N-CA	121.70	132.28	1
CD-NE-CZ	124.40	116.19	1
C-CA-CB	110.10	121.20	1
OE1-CD-NE2	122.60	116.79	1
C-N-CA	121.70	132.09	1
OE1-CD-NE2	122.60	116.86	1
C-N-CA	121.70	132.02	1
C-N-CA	121.70	131.98	1
C-N-CA	121.70	131.93	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
N-CA-C	111.00	126.76	1
C-N-CA	121.70	131.68	1
OE1-CD-NE2	122.60	117.07	1
C-N-CA	121.70	131.64	1
C-N-CA	121.70	131.58	1
OE1-CD-NE2	122.60	117.12	1
CA-CB-CG1	110.40	119.70	1
OE1-CD-NE2	122.60	117.13	1
OE1-CD-NE2	122.60	117.21	1
C-CA-CB	110.10	120.34	1
C-N-CA	121.70	131.40	1
C-N-CA	121.70	131.38	1
OD1-CG-ND2	122.60	117.22	1
CB-CG-ND1	122.70	130.69	1
N-CA-CB	111.50	102.49	1
OE1-CD-NE2	122.60	117.30	1
C-N-CA	121.70	131.24	1
C-N-CA	121.70	131.22	1
OE1-CD-NE2	122.60	117.31	1
N-CA-C	111.00	125.78	1
CD-NE-CZ	124.40	131.77	1
OE1-CD-NE2	122.60	117.34	2
C-N-CA	121.70	131.14	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
C-N-CA	121.70	131.12	1
OE1-CD-NE2	122.60	117.39	1
N-CA-CB	110.40	102.60	1
CA-CB-CG2	110.50	119.33	1
CA-C-N	116.20	126.57	1
C-N-CA	121.70	131.00	2
N-CA-CB	103.00	108.67	1
OE1-CD-NE2	122.60	117.47	1
C-N-CA	121.70	130.87	1
C-N-CA	121.70	130.84	1
OE1-CD-NE2	122.60	117.53	2
OE1-CD-NE2	122.60	117.56	1
CA-CB-CG2	110.50	119.06	1
OE1-CD-NE2	122.60	117.57	1
OE1-CD-NE2	122.60	117.59	1
N-CA-C	113.30	127.81	1
CA-CB-CG	112.60	117.57	1
OE1-CD-NE2	122.60	117.63	1
OE1-CD-NE2	122.60	117.64	2
C-N-CA	121.70	130.61	1
OE1-CD-NE2	122.60	117.65	1
C-CA-CB	110.10	119.49	1
CA-CB-CG	113.80	108.86	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.67	3
NE-CZ-NH2	119.20	123.63	1
CA-CB-CG	112.60	117.52	2
OE1-CD-NE2	122.60	117.69	4
OE1-CD-NE2	122.60	117.70	1
OE1-CD-NE2	122.60	117.71	1
CA-CB-CG	112.60	117.49	1
OE1-CD-NE2	122.60	117.72	2
OD1-CG-ND2	122.60	117.72	1
OE1-CD-NE2	122.60	117.73	1
CA-C-N	116.20	125.95	1
C-N-CA	121.70	130.47	1
OE1-CD-NE2	122.60	117.74	1
O-C-N	123.00	115.23	1
OE1-CD-NE2	122.60	117.75	1
C-CA-CB	110.10	119.32	1
C-N-CA	121.70	130.41	1
OE1-CD-NE2	122.60	117.76	1
OD1-CG-ND2	122.60	117.78	1
OE1-CD-NE2	122.60	117.79	1
OD1-CG-ND2	122.60	117.79	1
OE1-CD-NE2	122.60	117.81	2
OE1-CD-NE2	122.60	117.82	2

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.84	1
N-CA-CB	111.50	119.59	1
CA-CB-CG	112.60	117.36	1
C-N-CA	121.70	130.26	1
C-N-CA	121.70	130.25	1
OE1-CD-NE2	122.60	117.85	1
O-C-N	123.00	115.41	1
OE1-CD-NE2	122.60	117.88	1
C-N-CA	121.70	130.19	2
OE1-CD-NE2	122.60	117.89	1
C-N-CA	121.70	130.17	1
C-N-CA	121.70	130.14	1
OE1-CD-NE2	122.60	117.92	2
C-N-CA	121.70	130.13	1
OD1-CG-ND2	122.60	117.92	1
OD1-CG-ND2	122.60	117.93	1
OE1-CD-NE2	122.60	117.94	1
OD1-CG-ND2	122.60	117.94	1
CA-CB-CG	112.60	117.26	2
C-CA-CB	111.40	120.25	1
N-CA-CB	103.00	108.12	1
CA-CB-CG	113.80	118.45	1
CA-CB-CG	112.60	117.25	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
C-N-CA	121.70	130.05	1
OE1-CD-NE2	122.60	117.98	1
CA-CB-OG1	109.60	116.53	1
CG-CD-CE	111.30	100.68	1
OE1-CD-NE2	122.60	117.99	1
C-N-CA	121.70	129.99	1
OE1-CD-NE2	122.60	118.00	1
CB-CG-CD	112.60	104.78	1
C-N-CA	121.70	129.98	1
OE1-CD-NE2	122.60	118.01	1
CA-C-N	116.20	125.36	1
OE1-CD-NE2	122.60	118.02	1
CD1-CG-CD2	110.80	100.76	1
CA-CB-CG	112.60	117.16	1
OE1-CD-NE2	122.60	118.04	1
OE1-CD-NE2	122.60	118.05	2
C-N-CA	121.70	129.89	1
OD1-CG-ND2	122.60	118.05	1
OE1-CD-NE2	122.60	118.06	1
OE1-CD-NE2	122.60	118.07	2
C-N-CA	121.70	129.84	1
OE1-CD-NE2	122.60	118.08	1
CA-CB-CG1	110.40	118.08	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
CB-CG-CD2	131.20	125.33	1
OE1-CD-NE2	122.60	118.09	5
CB-CG-CD2	131.20	125.34	1
OE1-CD-NE2	122.60	118.10	2
OE1-CD-NE2	122.60	118.11	1
OD1-CG-ND2	122.60	118.11	1
OE1-CD-NE2	122.60	118.12	4
OE1-CD-NE2	122.60	118.13	3
C-CA-CB	110.50	117.21	1
OD1-CG-ND2	122.60	118.13	2
OE1-CD-NE2	122.60	118.14	1
CA-C-O	120.80	113.21	1
OE1-CD-NE2	122.60	118.15	1
OE1-CD-NE2	122.60	118.16	2
C-N-CA	121.70	129.68	1
OE1-CD-NE2	122.60	118.17	4
CA-C-N	116.20	125.05	1
OE1-CD-NE2	122.60	118.18	6
OE1-CD-NE2	122.60	118.19	2
C-N-CA	121.70	129.64	1
O-C-N	123.00	115.96	1
C-N-CA	121.70	129.62	1
C-CA-CB	110.10	118.45	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.20	1
N-CA-CB	110.50	103.03	1
OE1-CD-NE2	122.60	118.21	2
C-N-CA	121.70	129.60	1
CA-CB-CG2	110.40	102.94	1
OE1-CD-NE2	122.60	118.22	3
OE1-CD-NE2	122.60	118.23	1
CA-C-N	116.90	123.45	1
CA-CB-CG	112.60	116.97	2
OE1-CD-NE2	122.60	118.24	3
OD1-CG-ND2	122.60	118.25	1
C-N-CA	121.70	129.52	1
OE1-CD-NE2	122.60	118.26	2
C-CA-CB	110.10	118.34	1
OE1-CD-NE2	122.60	118.27	2
CA-CB-CG2	110.50	117.85	1
CB-CG-CD1	110.70	123.67	1
OE1-CD-NE2	122.60	118.28	3
OE1-CD-NE2	122.60	118.29	1
OE1-CD-NE2	122.60	118.30	1
OE1-CD-NE2	122.60	118.31	2
OE1-CD-NE2	122.60	118.32	3
N-CA-C	112.10	101.41	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.33	5
OE1-CD-NE2	122.60	118.34	6
CB-CG-CD2	131.20	125.66	1
CA-C-N	116.20	124.72	1
OE1-CD-NE2	122.60	118.35	5
CA-CB-CG	112.60	116.85	1
CA-CB-CG	114.10	122.59	1
CA-CB-CG	112.60	116.84	1
OE1-CD-NE2	122.60	118.36	3
CB-CG-CD2	131.20	125.69	1
CD-NE-CZ	124.40	130.33	2
CA-N-CD	112.00	106.07	1
N-CA-CB	103.00	107.66	1
OE1-CD-NE2	122.60	118.37	5
CA-CB-CG	113.80	109.57	1
OE1-CD-NE2	122.60	118.38	4
CB-CG-CD2	131.20	125.72	1
OE1-CD-NE2	122.60	118.39	2
CA-CB-CG2	110.40	117.55	1
CA-CB-CG	112.60	116.81	1
OE1-CD-NE2	122.60	118.40	2
C-N-CA	121.70	129.26	2
OE1-CD-NE2	122.60	118.41	4

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
CB-CG-CD2	131.20	125.75	1
C-N-CA	121.70	129.24	1
CA-C-N	116.20	124.57	1
N-CA-C	111.00	122.72	1
CB-CG-CD2	131.20	125.76	1
OE1-CD-NE2	122.60	118.42	2
CA-CB-CG	112.60	116.78	1
OD1-CG-ND2	122.60	118.42	1
CA-CB-CG	112.60	116.77	1
OE1-CD-NE2	122.60	118.43	1
C-N-CA	121.70	129.20	1
NE-CZ-NH1	121.50	125.66	1
OE1-CD-NE2	122.60	118.44	3
CA-CB-CG	112.60	116.75	1
CB-CG-CD2	131.20	125.80	1
OE1-CD-NE2	122.60	118.45	3
OE1-CD-NE2	122.60	118.46	3
CA-CB-CG2	110.40	117.44	1
OD1-CG-ND2	122.60	118.46	1
C-N-CA	121.70	129.14	2
OE1-CD-NE2	122.60	118.47	4
C-N-CA	121.70	129.13	1
OE1-CD-NE2	122.60	118.48	4

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.49	4
C-N-CA	121.70	129.10	1
OE1-CD-NE2	122.60	118.50	1
CD-NE-CZ	124.40	130.14	1
CB-CG-CD	112.60	119.56	1
C-N-CA	121.70	129.07	2
OE1-CD-NE2	122.60	118.51	5
C-N-CA	121.70	129.05	1
OE1-CD-NE2	122.60	118.52	4
OD1-CG-ND2	122.60	118.52	1
CA-CB-CG	113.80	117.88	1
N-CA-CB	103.00	107.49	1
CG-CD-CE	111.30	101.92	1
OE1-CD-NE2	122.60	118.53	2
O-C-N	123.00	116.48	1
CA-CB-CG2	110.50	117.42	1
N-CA-CB	110.50	103.59	1
CD-NE-CZ	124.40	130.09	1
OE1-CD-NE2	122.60	118.54	3
OE1-CD-NE2	122.60	118.55	5
CA-CB-OG1	109.60	115.68	1
CA-CB-CG2	110.50	117.38	1
OE1-CD-NE2	122.60	118.56	4

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.57	7
O-C-N	123.00	116.55	1
CB-CG-CD2	131.20	125.97	1
CA-CB-CG	112.60	116.63	1
OE1-CD-NE2	122.60	118.58	4
CA-CB-CG	113.80	117.82	1
OE1-CD-NE2	122.60	118.59	6
CA-CB-CG	112.60	116.60	1
CB-CG-CD2	131.20	126.00	1
OE1-CD-NE2	122.60	118.60	1
CZ-NH2-HH21	108.00	120.00	1
C-N-H	112.23	124.30	1
HZ1-NZ-HZ2	96.89	109.00	1
C-N-H	112.00	124.30	1
C-N-H	111.98	124.30	1
HZ1-NZ-HZ3	96.65	109.00	1
HZ1-NZ-HZ3	96.60	109.00	1
HZ1-NZ-HZ2	96.45	109.00	1
HZ2-NZ-HZ3	96.44	109.00	1
HZ1-NZ-HZ2	96.41	109.00	1
HH11-NH1-HH12	107.28	120.00	1
CB-CA-HA	96.26	109.00	1
HZ1-NZ-HZ3	96.24	109.00	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
C-CA-HA	96.17	109.00	1
N-CA-HA	97.00	110.00	1
HH21-NH2-HH22	106.87	120.00	1
HH21-NH2-HH22	106.65	120.00	1
C-N-H	110.87	124.30	1
CD1-CG-HG	94.51	108.00	1
C-CA-HA	95.41	109.00	1
CD-NE2-HE21	106.19	120.00	1
C-N-H	110.40	124.30	1
HH21-NH2-HH22	105.97	120.00	1
HZ1-NZ-HZ3	94.59	109.00	1
CG-ND2-HD21	105.44	120.00	1
HE21-NE2-HE22	105.12	120.00	1
HH11-NH1-HH12	104.80	120.00	1
СВ-СА-НА	93.40	109.00	1
C-N-H	107.01	124.30	1
C-CA-HA	89.06	109.00	1
C-N-H	102.86	124.30	1
N-CA-HA	87.70	110.00	1
C-N-H	98.02	124.30	1
NE2-CD2-HD2	155.87	126.40	1
CE1-NE2-HE2	84.74	125.50	1
ND1-CE1-HE1	31.94	125.80	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
NE2-CE1-HE1	24.62	125.80	1
CD2-NE2-HE2	19.02	125.50	1

Too-close contacts?

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.

Model ID	Clash score	Number of clashes
1	4.42	43
2	1.95	19
3	2.57	25
4	6.07	59
5	4.73	46
6	2.06	20
7	2.67	26
8	3.50	34
9	1.23	12
10	1.75	17

All 301 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:181:LEU:HD13	A:216:PHE:CE2	1.001
1	A:181:LEU:HD22	A:216:PHE:CE1	0.888
1	A:181:LEU:HD22	A:216:PHE:CZ	0.769
1	A:5:ILE:HG22	A:18:ILE:HG22	0.674
1	A:339:LEU:HB3	A:344:THR:HG22	0.667
1	A:339:LEU:HD21	A:353:VAL:HG11	0.552

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:549:GLN:HB3	A:598:LEU:HD21	0.542
1	A:181:LEU:HD13	A:216:PHE:CZ	0.532
1	A:181:LEU:CD2	A:216:PHE:CE1	0.527
1	A:173:THR:HG21	A:404:MET:CE	0.515
1	A:81:GLU:HB3	A:226:HIS:CE1	0.502
1	A:427:SER:HB3	A:468:GLY:HA2	0.501
1	A:177:LEU:HD23	A:181:LEU:HD11	0.498
1	A:378:GLN:OE1	A:391:LEU:HD13	0.493
1	A:547:ARG:HH22	A:573:GLU:CD	0.489
1	A:173:THR:HG21	A:404:MET:HE1	0.487
1	A:222:ASN:HD22	A:322:VAL:HB	0.474
1	A:351:LYS:HE2	A:355:GLU:OE1	0.469
1	A:214:LYS:O	A:408:MET:CE	0.466
1	A:549:GLN:CB	A:598:LEU:HD21	0.460
1	A:396:PRO:HD2	A:401:ILE:O	0.459
1	A:181:LEU:CD2	A:216:PHE:CZ	0.454
1	A:244:PHE:HB2	A:296:MET:HE2	0.453
1	A:193:TYR:CE1	A:195:LEU:HD21	0.442
1	A:59:VAL:CG1	A:257:LEU:HD13	0.440
1	A:331:VAL:HG13	A:357:PHE:HA	0.437
1	A:214:LYS:O	A:408:MET:HE1	0.436
1	A:438:ILE:CD1	A:488:ALA:CB	0.433
1	A:207:ILE:HG12	A:216:PHE:CE1	0.432

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:214:LYS:C	A:408:MET:SD	0.430
1	A:26:VAL:HB	A:34:ARG:HH21	0.429
1	A:419:PRO:HA	A:478:ILE:O	0.426
1	A:341:GLY:H	A:367:PRO:HB3	0.425
1	A:268:LYS:HE2	A:272:GLU:OE1	0.423
1	A:42:TYR:CD2	A:105:VAL:HG11	0.419
1	A:390:LEU:HD21	A:409:THR:H	0.419
1	A:378:GLN:CD	A:391:LEU:HD13	0.417
1	A:466:PRO:HD2	A:469:MET:HE2	0.416
1	A:548:LYS:HE2	A:552:GLU:OE1	0.416
1	A:173:THR:CB	A:404:MET:HE1	0.407
1	A:341:GLY:N	A:367:PRO:HB3	0.405
1	A:207:ILE:HG23	A:216:PHE:CZ	0.403
1	A:390:LEU:CD2	A:409:THR:H	0.402
2	A:252:LEU:HD21	A:296:MET:HE1	0.801
2	A:286:ILE:HG13	A:296:MET:HE2	0.647
2	A:252:LEU:HD21	A:296:MET:CE	0.627
2	A:239:TYR:CE2	A:304:LYS:HE3	0.530
2	A:547:ARG:HH22	A:573:GLU:CD	0.481
2	A:146:PHE:CD1	A:150:GLN:HB3	0.478
2	A:557:LEU:HD13	A:598:LEU:HD23	0.466
2	A:143:PRO:HD2	A:146:PHE:CD2	0.458
2	A:467:ARG:NH2	A:544:HIS:HB3	0.454

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:167:ARG:HH11	A:378:GLN:NE2	0.454
2	A:496:GLU:OE1	A:498:LYS:HE2	0.451
2	A:524:GLU:OE1	A:528:LYS:HE3	0.437
2	A:496:GLU:CD	A:498:LYS:CE	0.435
2	A:351:LYS:HE2	A:355:GLU:OE1	0.429
2	A:309:VAL:HG21	A:346:MET:HE1	0.426
2	A:5:ILE:HG22	A:18:ILE:HG22	0.417
2	A:268:LYS:HE2	A:272:GLU:OE1	0.416
2	A:467:ARG:CZ	A:544:HIS:CG	0.414
2	A:141:THR:HG21	A:371:VAL:HG12	0.410
3	A:485:HIS:CE1	A:500:THR:OG1	1.181
3	A:485:HIS:ND1	A:485:HIS:NE2	0.936
3	A:485:HIS:HE1	A:500:THR:OG1	0.907
3	A:485:HIS:CE1	A:485:HIS:NE2	0.756
3	A:103:VAL:HG13	A:104:GLU:H	0.607
3	A:88:ILE:N	A:605:GLN:HA	0.491
3	A:94:ILE:H	A:609:GLN:H	0.486
3	A:86:VAL:N	A:605:GLN:H	0.477
3	A:70:LYS:HE2	A:143:PRO:HD3	0.474
3	A:85:ASP:O	A:606:HIS:HB3	0.474
3	A:87:SER:CB	A:604:GLN:HA	0.467
3	A:485:HIS:CE1	A:500:THR:CB	0.462
3	A:84:ARG:HA	A:602:ALA:HB1	0.459

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:485:HIS:CE1	A:500:THR:HG1	0.455
3	A:95:ALA:HB1	A:99:GLY:HA2	0.452
3	A:93:ILE:HD12	A:606:HIS:CD2	0.447
3	A:125:LYS:HZ2	A:129:ASP:CG	0.441
3	A:93:ILE:HD11	A:103:VAL:CG2	0.437
3	A:92:LYS:HB2	A:608:GLN:H	0.433
3	A:411:LEU:HD23	A:412:ILE:H	0.428
3	A:445:ARG:CB	A:448:ALA:HB2	0.422
3	A:485:HIS:CE1	A:500:THR:CG2	0.415
3	A:70:LYS:HZ1	A:171:GLU:CD	0.408
3	A:289:ASP:CG	A:294:LYS:HE2	0.407
3	A:85:ASP:O	A:605:GLN:CA	0.400
4	A:14:SER:HB2	A:123:MET:HE1	0.838
4	A:23:THR:HG22	A:24:PRO:HG3	0.768
4	A:14:SER:CB	A:123:MET:HE1	0.746
4	A:66:LEU:HD22	A:115:ILE:HG23	0.697
4	A:25:ARG:HE	A:49:LEU:HD13	0.688
4	A:23:THR:HG21	A:46:GLY:C	0.631
4	A:24:PRO:HA	A:43:THR:H	0.600
4	A:426:PHE:CD2	A:474:VAL:HB	0.591
4	A:66:LEU:CD2	A:115:ILE:HG23	0.578
4	A:119:VAL:HG12	A:123:MET:HE3	0.573
4	A:85:ASP:HB3	A:89:MET:HE3	0.572

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:173:THR:HG21	A:391:LEU:HD21	0.570
4	A:442:GLN:HE22	A:518:ASP:HB2	0.567
4	A:411:LEU:HD23	A:429:ALA:HB1	0.555
4	A:23:THR:HG21	A:46:GLY:O	0.551
4	A:23:THR:C	A:43:THR:H	0.544
4	A:69:ILE:HD13	A:115:ILE:HD13	0.540
4	A:442:GLN:HB2	A:515:MET:HE3	0.529
4	A:24:PRO:HA	A:42:TYR:HA	0.528
4	A:23:THR:HG22	A:24:PRO:CG	0.519
4	A:19:MET:SD	A:380:GLY:HA3	0.516
4	A:286:ILE:HD12	A:296:MET:HE1	0.511
4	A:177:LEU:HD11	A:391:LEU:CD1	0.491
4	A:24:PRO:CD	A:47:GLU:O	0.484
4	A:65:THR:HG23	A:91:PHE:CD1	0.478
4	A:24:PRO:CG	A:48:THR:HA	0.477
4	A:69:ILE:HG12	A:103:VAL:HG21	0.469
4	A:91:PHE:CE2	A:93:ILE:HD11	0.460
4	A:177:LEU:HD11	A:391:LEU:HD11	0.457
4	A:119:VAL:CG1	A:123:MET:HE3	0.452
4	A:24:PRO:CA	A:43:THR:H	0.451
4	A:286:ILE:HD12	A:296:MET:CE	0.450
4	A:24:PRO:HA	A:43:THR:N	0.449
4	A:17:ALA:CB	A:376:ALA:HB2	0.446

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:24:PRO:HG3	A:48:THR:HA	0.444
4	A:181:LEU:HD11	A:377:VAL:HG13	0.440
4	A:23:THR:C	A:43:THR:N	0.439
4	A:27:LEU:HD12	A:130:TYR:CD2	0.436
4	A:24:PRO:CA	A:42:TYR:HA	0.434
4	A:69:ILE:CD1	A:103:VAL:HG21	0.434
4	A:31:GLU:C	A:33:ASP:H	0.432
4	A:268:LYS:HE2	A:272:GLU:OE1	0.431
4	A:69:ILE:CD1	A:115:ILE:HG21	0.430
4	A:17:ALA:HB3	A:376:ALA:HB2	0.426
4	A:25:ARG:HE	A:49:LEU:CD1	0.426
4	A:72:LEU:HD11	A:93:ILE:HD12	0.424
4	A:351:LYS:HE2	A:355:GLU:OE1	0.424
4	A:27:LEU:CD1	A:130:TYR:CD2	0.419
4	A:23:THR:HB	A:46:GLY:CA	0.416
4	A:447:ARG:CZ	A:526:ASP:OD1	0.409
4	A:82:VAL:O	A:86:VAL:HG23	0.408
4	A:22:THR:O	A:23:THR:HB	0.408
4	A:190:ILE:HG22	A:336:ASP:HB2	0.407
4	A:239:TYR:CE2	A:304:LYS:HE2	0.406
4	A:65:THR:HG23	A:91:PHE:HD1	0.404
4	A:496:GLU:OE1	A:498:LYS:HE2	0.404
4	A:23:THR:CB	A:24:PRO:HD3	0.403

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:23:THR:OG1	A:47:GLU:N	0.403
4	A:24:PRO:N	A:43:THR:H	0.402
5	A:232:PHE:CE1	A:346:MET:HE1	0.794
5	A:69:ILE:HG22	A:397:LEU:HD22	0.782
5	A:69:ILE:CG2	A:397:LEU:HD22	0.781
5	A:116:SER:OG	A:397:LEU:HD21	0.664
5	A:396:PRO:C	A:397:LEU:HG	0.653
5	A:181:LEU:CD1	A:377:VAL:HG21	0.602
5	A:69:ILE:HG22	A:397:LEU:HB3	0.589
5	A:145:TYR:CE2	A:225:THR:HG23	0.568
5	A:436:VAL:HG21	A:472:ILE:HG13	0.564
5	A:167:ARG:HH11	A:382:LEU:HD21	0.552
5	A:39:ILE:HG22	A:130:TYR:CE2	0.539
5	A:181:LEU:HD11	A:377:VAL:HG11	0.523
5	A:5:ILE:HD11	A:130:TYR:CD1	0.520
5	A:64:ASN:HD21	A:403:THR:HG23	0.518
5	A:67:PHE:CG	A:89:MET:SD	0.515
5	A:73:ILE:HD11	A:397:LEU:HD11	0.515
5	A:115:ILE:HG21	A:399:LEU:HD11	0.508
5	A:150:GLN:HE22	A:225:THR:HG21	0.507
5	A:70:LYS:HA	A:397:LEU:HD12	0.506
5	A:139:VAL:HB	A:390:LEU:HD12	0.506
5	A:375:ALA:HB1	A:392:LEU:CD2	0.501

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:167:ARG:NH1	A:382:LEU:HD21	0.498
5	A:73:ILE:HD11	A:397:LEU:CD1	0.493
5	A:3:LYS:NZ	A:42:TYR:CD2	0.489
5	A:447:ARG:NH1	A:533:VAL:HG21	0.487
5	A:120:LEU:CD2	A:394:VAL:HG11	0.486
5	A:145:TYR:HE2	A:225:THR:HG23	0.486
5	A:5:ILE:HD11	A:130:TYR:CE1	0.484
5	A:375:ALA:C	A:390:LEU:HD21	0.484
5	A:181:LEU:HD11	A:377:VAL:HG21	0.476
5	A:412:ILE:HD11	A:476:PHE:CD2	0.459
5	A:375:ALA:CB	A:392:LEU:HD22	0.442
5	A:69:ILE:HG21	A:115:ILE:HG21	0.440
5	A:120:LEU:HD21	A:394:VAL:HG11	0.435
5	A:375:ALA:HB1	A:392:LEU:HD22	0.433
5	A:4:ILE:HD13	A:380:GLY:N	0.428
5	A:66:LEU:HD12	A:399:LEU:HB3	0.422
5	A:69:ILE:HG22	A:397:LEU:CD2	0.417
5	A:4:ILE:CD1	A:380:GLY:HA2	0.416
5	A:239:TYR:CE2	A:304:LYS:HE2	0.416
5	A:16:VAL:CG2	A:37:PRO:CG	0.412
5	A:232:PHE:CD1	A:346:MET:HE1	0.412
5	A:351:LYS:HE2	A:355:GLU:OE1	0.409
5	A:116:SER:HG	A:397:LEU:HD21	0.401

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:39:ILE:CG2	A:130:TYR:CD2	0.400
5	A:421:LYS:HE3	A:475:THR:HG21	0.400
6	A:73:ILE:HG23	A:153:ALA:HB3	0.613
6	A:394:VAL:CG1	A:415:ASN:HA	0.593
6	A:73:ILE:HG23	A:153:ALA:CB	0.556
6	A:68:ALA:HB1	A:71:ARG:HH21	0.550
6	A:141:THR:HG21	A:371:VAL:HG12	0.508
6	A:399:LEU:HD12	A:478:ILE:HD11	0.472
6	A:547:ARG:HH22	A:573:GLU:CD	0.454
6	A:37:PRO:HA	A:369:GLU:OE1	0.450
6	A:181:LEU:CD1	A:377:VAL:HG21	0.443
6	A:23:THR:HG23	A:42:TYR:O	0.442
6	A:73:ILE:HG22	A:150:GLN:HA	0.442
6	A:351:LYS:HE2	A:355:GLU:OE1	0.441
6	A:548:LYS:HE2	A:552:GLU:OE1	0.440
6	A:565:ILE:HD13	A:598:LEU:HD11	0.439
6	A:244:PHE:HB2	A:296:MET:HE2	0.434
6	A:5:ILE:HG22	A:18:ILE:HG22	0.431
6	A:496:GLU:OE1	A:498:LYS:HE2	0.418
6	A:202:ILE:HG12	A:320:LEU:HD23	0.415
6	A:496:GLU:CD	A:498:LYS:HE2	0.413
6	A:68:ALA:CB	A:89:MET:HE1	0.409
7	A:232:PHE:CE1	A:346:MET:HE1	0.706

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:395:THR:C	A:416:THR:HG21	0.704
7	A:396:PRO:HB3	A:414:LYS:HA	0.675
7	A:407:VAL:HG23	A:448:ALA:HB2	0.675
7	A:394:VAL:C	A:416:THR:HB	0.655
7	A:399:LEU:HD12	A:412:ILE:HD12	0.637
7	A:179:TYR:CE2	A:338:ILE:HG23	0.562
7	A:467:ARG:HH22	A:540:ASP:CG	0.554
7	A:401:ILE:HD11	A:474:VAL:HG11	0.546
7	A:407:VAL:HG21	A:441:LEU:CD1	0.546
7	A:232:PHE:CD1	A:346:MET:HE1	0.541
7	A:395:THR:O	A:416:THR:HG21	0.540
7	A:103:VAL:HG22	A:115:ILE:HD11	0.537
7	A:396:PRO:CB	A:414:LYS:HA	0.510
7	A:410:THR:HG21	A:422:HIS:CD2	0.497
7	A:394:VAL:HB	A:416:THR:HB	0.467
7	A:421:LYS:HE3	A:475:THR:HG21	0.455
7	A:419:PRO:HA	A:478:ILE:O	0.453
7	A:5:ILE:HG22	A:18:ILE:HG22	0.450
7	A:442:GLN:HB2	A:454:LEU:HD11	0.447
7	A:351:LYS:HE2	A:355:GLU:OE1	0.444
7	A:547:ARG:HH22	A:573:GLU:CD	0.441
7	A:218:VAL:O	A:480:ALA:HB1	0.438
7	A:407:VAL:HG23	A:448:ALA:CB	0.426

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:407:VAL:CG2	A:448:ALA:HB2	0.420
7	A:268:LYS:HE2	A:272:GLU:OE1	0.401
8	A:244:PHE:HB2	A:296:MET:HE2	0.690
8	A:557:LEU:HD11	A:598:LEU:HD21	0.644
8	A:258:ALA:HB2	A:285:TYR:CE2	0.592
8	A:29:ASN:HD21	A:36:THR:CB	0.574
8	A:39:ILE:HD11	A:55:LYS:HA	0.574
8	A:258:ALA:HB2	A:285:TYR:HE2	0.551
8	A:219:LEU:HA	A:480:ALA:HB1	0.544
8	A:547:ARG:HH22	A:573:GLU:CD	0.538
8	A:51:GLY:HA3	A:122:LYS:HZ2	0.502
8	A:25:ARG:NH1	A:130:TYR:CE2	0.485
8	A:39:ILE:CD1	A:55:LYS:HA	0.483
8	A:351:LYS:HE2	A:355:GLU:OE1	0.474
8	A:145:TYR:CZ	A:222:ASN:C	0.472
8	A:395:THR:HG22	A:397:LEU:O	0.468
8	A:239:TYR:CE2	A:304:LYS:HE2	0.461
8	A:467:ARG:NH2	A:544:HIS:HB3	0.457
8	A:69:ILE:CD1	A:115:ILE:HG21	0.456
8	A:12:THR:HG23	A:67:PHE:CZ	0.454
8	A:29:ASN:HD21	A:36:THR:HB	0.454
8	A:44:GLN:O	A:106:LYS:HE3	0.452
8	A:244:PHE:CE1	A:252:LEU:HD21	0.448

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:394:VAL:CG1	A:415:ASN:HA	0.444
8	A:5:ILE:HG22	A:18:ILE:HG22	0.442
8	A:123:MET:HA	A:123:MET:HE2	0.440
8	A:378:GLN:OE1	A:391:LEU:HD12	0.440
8	A:145:TYR:OH	A:221:THR:HB	0.432
8	A:244:PHE:CB	A:296:MET:HE2	0.430
8	A:557:LEU:HD11	A:598:LEU:CD2	0.430
8	A:268:LYS:HE2	A:272:GLU:OE1	0.422
8	A:12:THR:HG23	A:67:PHE:HZ	0.420
8	A:45:ASP:C	A:106:LYS:HE3	0.417
8	A:41:ALA:HB1	A:65:THR:HG23	0.410
8	A:51:GLY:HA3	A:122:LYS:NZ	0.405
8	A:467:ARG:NH2	A:544:HIS:CB	0.402
9	A:179:TYR:CE2	A:338:ILE:HG23	0.546
9	A:462:ILE:HG21	A:472:ILE:HD11	0.520
9	A:440:VAL:HG12	A:515:MET:HE1	0.517
9	A:548:LYS:HE2	A:552:GLU:OE1	0.479
9	A:351:LYS:HE2	A:355:GLU:OE1	0.472
9	A:440:VAL:CG1	A:515:MET:HE1	0.453
9	A:244:PHE:HB2	A:296:MET:HE2	0.452
9	A:14:SER:H	A:37:PRO:HG3	0.445
9	A:423:SER:HB2	A:473:GLU:CG	0.444
9	A:148:ASP:OD1	A:399:LEU:HD23	0.433

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:42:TYR:CD2	A:105:VAL:HG11	0.424
9	A:547:ARG:HH22	A:573:GLU:CD	0.415
10	A:252:LEU:HD21	A:296:MET:HE1	0.812
10	A:145:TYR:CE2	A:225:THR:HG22	0.584
10	A:320:LEU:HD22	A:356:PHE:CE1	0.513
10	A:268:LYS:HE2	A:272:GLU:OE1	0.503
10	A:285:TYR:HB2	A:296:MET:HE2	0.493
10	A:103:VAL:HG22	A:115:ILE:HD11	0.483
10	A:351:LYS:HE2	A:355:GLU:OE1	0.475
10	A:262:LEU:HD13	A:283:LEU:HD11	0.457
10	A:179:TYR:O	A:183:LYS:HE2	0.445
10	A:185:THR:HG22	A:209:GLU:OE2	0.440
10	A:179:TYR:CE2	A:183:LYS:HE3	0.439
10	A:213:GLU:HA	A:388:ASP:HB3	0.429
10	A:547:ARG:HH22	A:573:GLU:CD	0.426
10	A:565:ILE:HD13	A:598:LEU:CD1	0.425
10	A:411:LEU:HD12	A:476:PHE:CE2	0.415
10	A:244:PHE:CE2	A:283:LEU:HD12	0.409
10	A:548:LYS:HE2	A:552:GLU:OE1	0.400

Torsion angles: Protein backbone?

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	636	609	18	9

Model ID	Analyzed	Favored	Allowed	Outliers
2	636	613	19	4
3	636	619	13	4
4	636	565	58	13
5	636	600	20	16
6	636	598	28	10
7	636	610	17	9
8	636	610	19	7
9	636	607	22	7
10	636	606	21	9

Detailed list of outliers are tabulated below.

Torsion angles: Protein sidechains ?

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	521	498	12	11
2	521	507	11	3
3	521	449	42	30
4	521	493	15	13
5	521	495	13	13
6	521	502	13	6
7	521	504	10	7
8	521	499	17	5
9	521	495	22	4
10	521	505	13	3

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	225	THR
1	A	340	VAL
1	A	367	PRO
1	A	409	THR
1	A	411	LEU
1	A	416	THR
1	A	417	THR
1	A	420	THR
1	А	469	MET
1	A	598	LEU
1	А	625	ASP
2	A	1	MET
2	A	287	THR
2	А	544	HIS
3	А	12	THR
3	А	33	ASP
3	A	45	ASP
3	A	57	GLN
3	A	78	GLN
3	A	85	ASP
3	A	86	VAL
3	A	87	SER
3	A	94	ILE

Model ID	Chain	Residue ID	Residue type
3	А	97	ASP
3	А	104	GLU
3	А	189	THR
3	А	304	LYS
3	А	332	SER
3	А	340	VAL
3	А	388	ASP
3	A	394	VAL
3	А	397	LEU
3	А	399	LEU
3	А	411	LEU
3	А	412	ILE
3	А	428	THR
3	А	467	ARG
3	А	508	ASN
3	А	548	LYS
3	А	605	GLN
3	A	611	THR
3	А	620	ASN
3	А	623	ASP
3	A	631	PHE
4	A	1	MET
4	А	14	SER

Model ID	Chain	Residue ID	Residue type
4	A	23	THR
4	A	24	PRO
4	A	43	THR
4	A	60	THR
4	А	123	MET
4	А	395	THR
4	А	402	GLU
4	A	409	THR
4	A	410	THR
4	A	611	THR
4	A	625	ASP
5	A	36	THR
5	А	38	SER
5	А	39	ILE
5	А	42	TYR
5	А	65	THR
5	А	386	VAL
5	A	394	VAL
5	A	395	THR
5	A	399	LEU
5	A	417	THR
5	A	420	THR
5	A	543	LEU

Model ID	Chain	Residue ID	Residue type
5	A	611	THR
6	A	50	VAL
6	А	60	THR
6	А	65	THR
6	А	367	PRO
6	A	420	THR
6	А	557	LEU
7	А	1	MET
7	А	393	ASP
7	A	416	THR
7	A	417	THR
7	A	436	VAL
7	А	606	HIS
7	А	611	THR
8	А	394	VAL
8	А	417	THR
8	A	611	THR
8	A	615	ASP
8	A	636	ASP
9	A	215	THR
9	A	395	THR
9	A	410	THR
9	A	636	ASP

Model ID	Chain	Residue ID	Residue type
10	А	283	LEU
10	А	298	ILE
10	А	420	THR

Fit of model to data used for modeling @

Crosslinking-MS

Validation for this section is under development.

Fit of model to data used for validation @

Validation for this section is under development.

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